Full wwPDB X-ray Structure Validation Report (i)

Aug 20, 2023 – 03:17 PM EDT

PDB ID	:	2NY2
Title	:	HIV-1 gp120 Envelope Glycoprotein (T123C, T257S, S334A, S375W, G431C) Complexed with CD4 and Antibody 17b
Authors	:	Zhou, T.; Xu, L.; Dey, B.; Hessell, A.J.; Van Ryk, D.; Xiang, S.H.; Yang, X.; Zhang, M.Y.; Zwick, M.B.; Arthos, J.; Burton, D.R.; Dimitrov, D.S.; Sodroski, J.; Wyatt, R.; Nabel, G.J.; Kwong, P.D.
Deposited on	:	2006-11-20
Resolution	:	2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

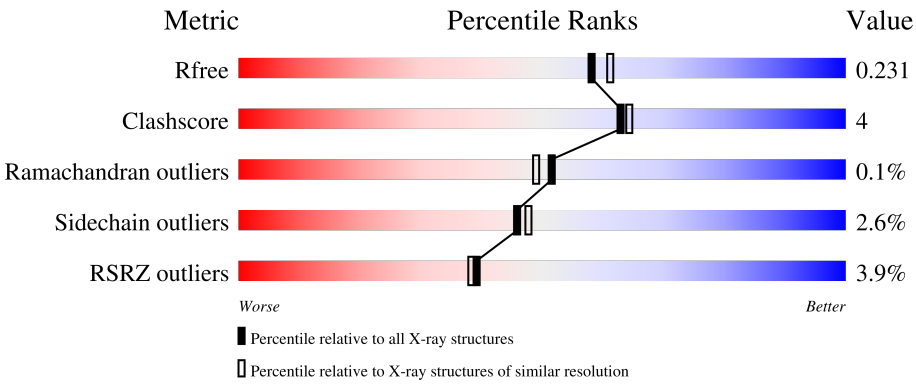
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	317	6%, 85%, 9%
2	B	184	7%, 89%, 9%
3	C	214	%, 89%, 10%
4	D	229	86%, 10%

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Mol	Chain	Length	Quality of chain
5	E	2	50% 50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	NAG	A	730	-	-	-	X
6	NAG	A	734	-	-	-	X
6	NAG	A	741	-	-	-	X
6	NAG	A	762	-	-	-	X
6	NAG	A	776	-	-	-	X
6	NAG	A	789	-	-	-	X
6	NAG	A	795	-	-	-	X
6	NAG	A	886	-	-	-	X
6	NAG	A	892	-	-	-	X
6	NAG	A	948	-	-	-	X
7	EDO	A	4001	-	-	-	X
8	HEZ	A	4003	-	-	-	X

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 7945 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ENVELOPE GLYCOPROTEIN GP120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	304	2358	1482	411	443	22	0	0	0

- Molecule 2 is a protein called T-cell surface glycoprotein CD4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	181	1412	885	247	276	4	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1000	MET	-	initiating methionine	UNP P01730

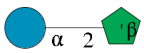
- Molecule 3 is a protein called ANTIBODY 17B, LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	214	1646	1028	282	331	5	0	0	0

- Molecule 4 is a protein called ANTIBODY 17B, HEAVY CHAIN.

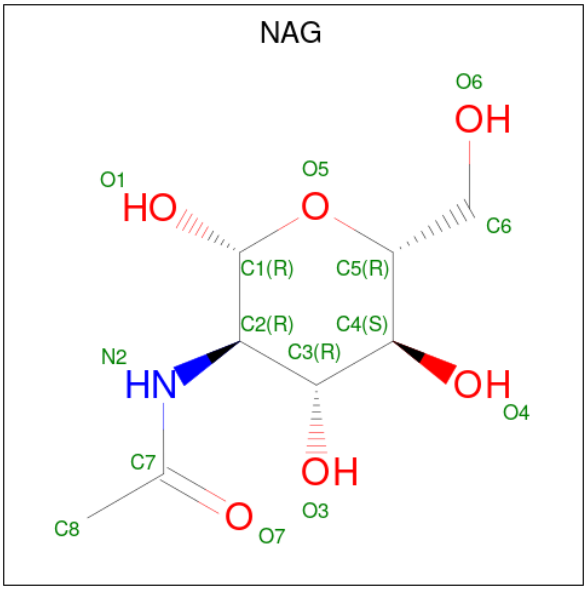
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	221	1671	1057	280	329	5	0	1	0

- Molecule 5 is an oligosaccharide called beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	O				
5	E	2	23	12	11		0	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	A	1	14	8	1	5	0	0
			Total	C	N	O		
6	A	1	14	8	1	5	0	0
			Total	C	N	O		
6	A	1	14	8	1	5	0	0
			Total	C	N	O		
6	A	1	14	8	1	5	0	0
			Total	C	N	O		
6	A	1	14	8	1	5	0	0
			Total	C	N	O		
6	A	1	14	8	1	5	0	0
			Total	C	N	O		
6	A	1	14	8	1	5	0	0
			Total	C	N	O		
6	A	1	14	8	1	5	0	0
			Total	C	N	O		
6	A	1	14	8	1	5	0	0
			Total	C	N	O		
6	A	1	14	8	1	5	0	0

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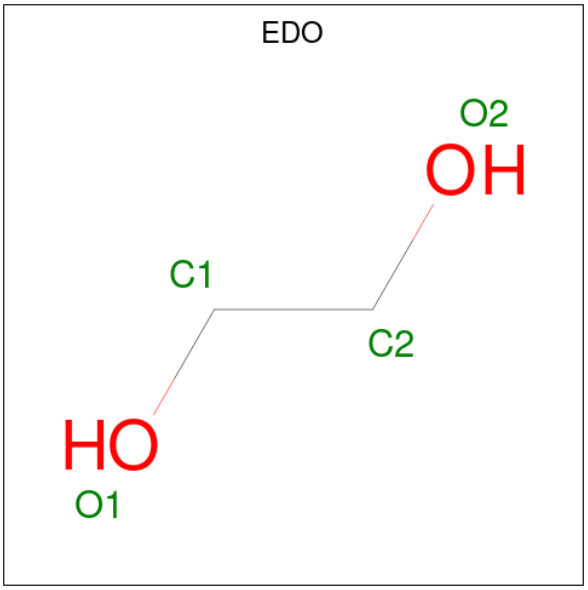
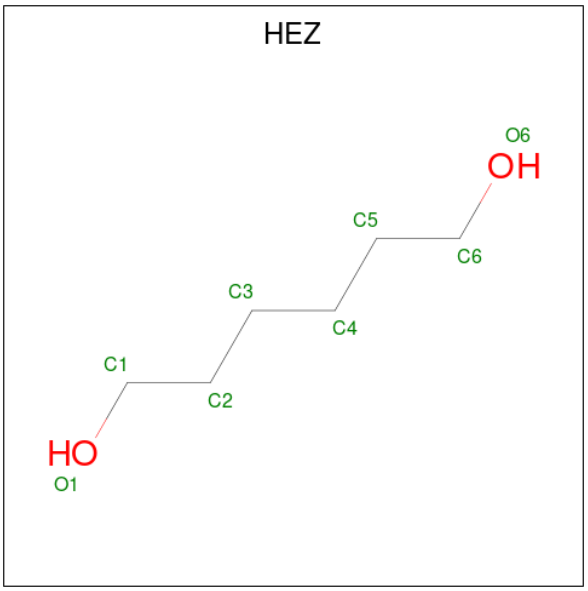
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	A	1	14	8	1	5	0	0

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
7	A	1	4	2	2		0	0
7	D	1	Total	C	O		0	0
			4	2	2			

- Molecule 8 is HEXANE-1,6-DIOL (three-letter code: HEZ) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	A	1	8	6	2	0	0

- Molecule 9 is water.

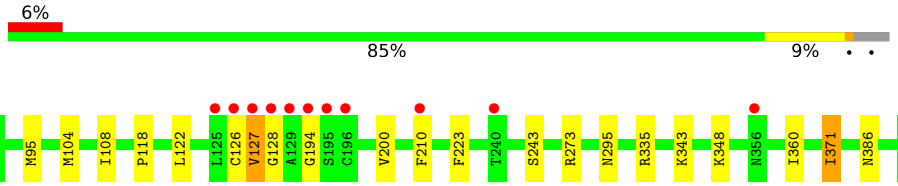
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	204	204	204	0	0
			Total	O		
9	B	98	98	98	0	0
			Total	O		
9	C	164	164	164	0	0
			Total	O		
9	D	199	199	199	0	0

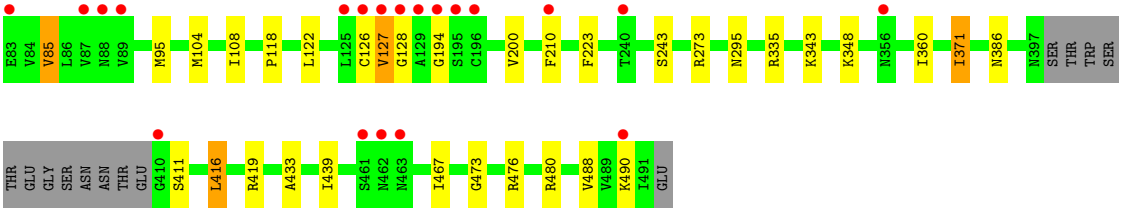
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: ENVELOPE GLYCOPROTEIN GP120

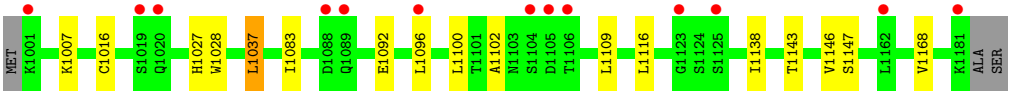
Chain A:





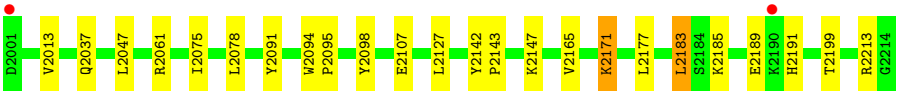
• Molecule 2: T-cell surface glycoprotein CD4

Chain B:



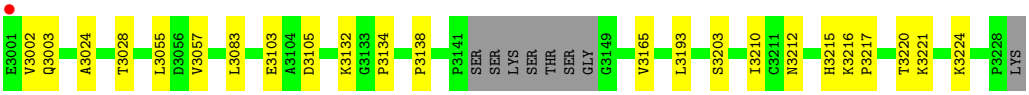
• Molecule 3: ANTIBODY 17B, LIGHT CHAIN

Chain C:



• Molecule 4: ANTIBODY 17B, HEAVY CHAIN

Chain D:



• Molecule 5: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain E:

GLC1
FRU2

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	71.61Å 88.02Å 196.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.84 – 2.00 42.82 – 2.00	Depositor EDS
% Data completeness (in resolution range)	94.6 (42.84-2.00) 94.6 (42.82-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.08 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.194 , 0.223 0.209 , 0.231	Depositor DCC
R_{free} test set	4062 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	28.7	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 56.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7945	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: HEZ, FRU, NAG, EDO, GLC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.29	0/2406	0.46	0/3263
2	B	0.27	0/1432	0.46	1/1930 (0.1%)
3	C	0.29	0/1683	0.49	0/2288
4	D	0.31	0/1716	0.50	0/2339
All	All	0.29	0/7237	0.47	1/9820 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1037	LEU	CA-CB-CG	5.57	128.12	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2358	0	2304	24	0
2	B	1412	0	1441	6	0
3	C	1646	0	1590	15	0
4	D	1671	0	1631	16	0
5	E	23	0	21	1	0
6	A	154	0	143	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	4	0	6	0	0
7	D	4	0	6	0	0
8	A	8	0	14	0	0
9	A	204	0	0	5	1
9	B	98	0	0	0	0
9	C	164	0	0	2	0
9	D	199	0	0	6	0
All	All	7945	0	7156	62	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (62) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:3212:ASN:ND2	9:D:240:HOH:O	1.89	1.00
3:C:2191:HIS:O	3:C:2213:ARG:NH1	1.97	0.98
4:D:3215:HIS:HB3	4:D:3220:THR:HG22	1.54	0.89
4:D:3210:ILE:HG22	9:D:240:HOH:O	1.83	0.79
3:C:2185:LYS:HE2	3:C:2189:GLU:OE2	1.89	0.72
4:D:3215:HIS:HB3	4:D:3220:THR:CG2	2.20	0.72
6:A:839:NAG:O7	9:A:4205:HOH:O	2.10	0.69
1:A:122:LEU:HD22	1:A:200:VAL:HG22	1.75	0.67
1:A:122:LEU:HD21	4:D:3057:VAL:HG21	1.76	0.67
1:A:411:SER:OG	9:A:4123:HOH:O	2.14	0.65
1:A:371:ILE:HD11	1:A:473:GLY:CA	2.29	0.63
1:A:419:ARG:NH1	9:A:4079:HOH:O	2.32	0.63
2:B:1138:ILE:HG21	2:B:1146:VAL:HG22	1.82	0.60
4:D:3134:PRO:HD2	4:D:3220:THR:HG21	1.83	0.60
2:B:1083:ILE:HG13	2:B:1092:GLU:HG3	1.83	0.59
1:A:419:ARG:NH1	4:D:3103:GLU:OE2	2.33	0.57
3:C:2183:LEU:N	3:C:2183:LEU:HD23	2.20	0.55
3:C:2171:LYS:HA	3:C:2171:LYS:HE3	1.87	0.55
1:A:386:ASN:O	1:A:416:LEU:HG	2.07	0.54
1:A:335:ARG:NH2	9:A:4103:HOH:O	2.21	0.54
1:A:371:ILE:HD11	1:A:473:GLY:HA3	1.90	0.54
3:C:2094:TRP:HA	3:C:2095:PRO:C	2.29	0.52
1:A:223:PHE:HB3	1:A:488:VAL:HG13	1.91	0.52
3:C:2147:LYS:HB3	3:C:2199:THR:HB	1.91	0.51
3:C:2165:VAL:HG22	3:C:2177:LEU:HD12	1.93	0.51
4:D:3002:VAL:HG21	4:D:3024:ALA:HB1	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2091:TYR:HA	3:C:2098:TYR:CD1	2.47	0.49
1:A:210:PHE:HB3	9:A:4179:HOH:O	2.11	0.49
1:A:126:CYS:O	1:A:127:VAL:HB	2.14	0.47
1:A:360:ILE:HB	1:A:467:ILE:HD13	1.96	0.46
9:D:45:HOH:O	5:E:2:FRU:O1	2.18	0.46
1:A:104:MET:O	1:A:108:ILE:HG12	2.16	0.46
3:C:2075:ILE:HG22	9:C:340:HOH:O	2.15	0.46
4:D:3105:ASP:OD1	4:D:3105:ASP:N	2.49	0.46
3:C:2037:GLN:HB2	3:C:2047:LEU:HD11	1.98	0.46
1:A:371:ILE:HD11	1:A:473:GLY:HA2	1.95	0.45
1:A:295:ASN:HD22	6:A:795:NAG:H83	1.81	0.45
3:C:2061:ARG:HB2	9:C:340:HOH:O	2.15	0.45
1:A:343:LYS:HE3	6:A:839:NAG:H82	1.97	0.45
1:A:128:GLY:C	1:A:194:GLY:H	2.20	0.45
6:A:839:NAG:O7	6:A:839:NAG:C1	2.65	0.45
3:C:2183:LEU:HD23	3:C:2183:LEU:H	1.82	0.44
4:D:3216:LYS:N	4:D:3217:PRO:CD	2.81	0.44
1:A:85:VAL:HA	1:A:243:SER:HB3	2.00	0.44
2:B:1102:ALA:HA	2:B:1116:LEU:HD23	2.01	0.43
1:A:343:LYS:HE3	6:A:839:NAG:C8	2.49	0.43
2:B:1007:LYS:HG3	2:B:1168:VAL:HG21	2.01	0.42
3:C:2142:TYR:CG	3:C:2143:PRO:HA	2.55	0.42
3:C:2183:LEU:N	3:C:2183:LEU:CD2	2.83	0.42
1:A:95:MET:SD	1:A:273:ARG:HD3	2.60	0.41
1:A:348:LYS:HD3	1:A:348:LYS:HA	1.90	0.41
1:A:476:ARG:O	1:A:480:ARG:HB2	2.20	0.41
2:B:1016:CYS:HB2	2:B:1028:TRP:CZ2	2.56	0.41
4:D:3003:GLN:NE2	9:D:279:HOH:O	2.54	0.41
4:D:3003:GLN:NE2	9:D:372:HOH:O	2.53	0.41
4:D:3132:LYS:HE3	4:D:3132:LYS:HB2	1.95	0.41
1:A:118:PRO:HB3	1:A:433:ALA:HB1	2.03	0.41
4:D:3138:PRO:HD3	4:D:3224:LYS:HE2	2.03	0.41
2:B:1138:ILE:HD13	2:B:1146:VAL:HG23	2.03	0.40
3:C:2013:VAL:CG1	3:C:2078:LEU:HD12	2.52	0.40
4:D:3221:LYS:NZ	9:D:614:HOH:O	2.53	0.40
4:D:3193:LEU:C	4:D:3193:LEU:HD12	2.42	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:4171:HOH:O	9:A:4171:HOH:O[4_556]	1.30	0.90

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	300/317 (95%)	286 (95%)	13 (4%)	1 (0%)	41	37
2	B	179/184 (97%)	173 (97%)	6 (3%)	0	100	100
3	C	212/214 (99%)	205 (97%)	7 (3%)	0	100	100
4	D	218/229 (95%)	214 (98%)	4 (2%)	0	100	100
All	All	909/944 (96%)	878 (97%)	30 (3%)	1 (0%)	51	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	127	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	269/281 (96%)	264 (98%)	5 (2%)	57	61
2	B	164/166 (99%)	157 (96%)	7 (4%)	29	26
3	C	184/184 (100%)	180 (98%)	4 (2%)	52	55
4	D	187/193 (97%)	182 (97%)	5 (3%)	44	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	804/824 (98%)	783 (97%)	21 (3%)	46 48

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	VAL
1	A	371	ILE
1	A	416	LEU
1	A	439	ILE
1	A	490	LYS
2	B	1027	HIS
2	B	1037	LEU
2	B	1096	LEU
2	B	1100	LEU
2	B	1109	LEU
2	B	1143	THR
2	B	1147	SER
3	C	2107	GLU
3	C	2127	LEU
3	C	2171	LYS
3	C	2183	LEU
4	D	3028	THR
4	D	3055	LEU
4	D	3083	LEU
4	D	3165	VAL
4	D	3203	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	1073	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

2 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	GLC	E	1	5	11,11,12	0.61	0	15,15,17	0.73	0
5	FRU	E	2	5	11,12,12	0.49	0	10,18,18	0.62	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GLC	E	1	5	-	1/2/19/22	0/1/1/1
5	FRU	E	2	5	-	5/5/24/24	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

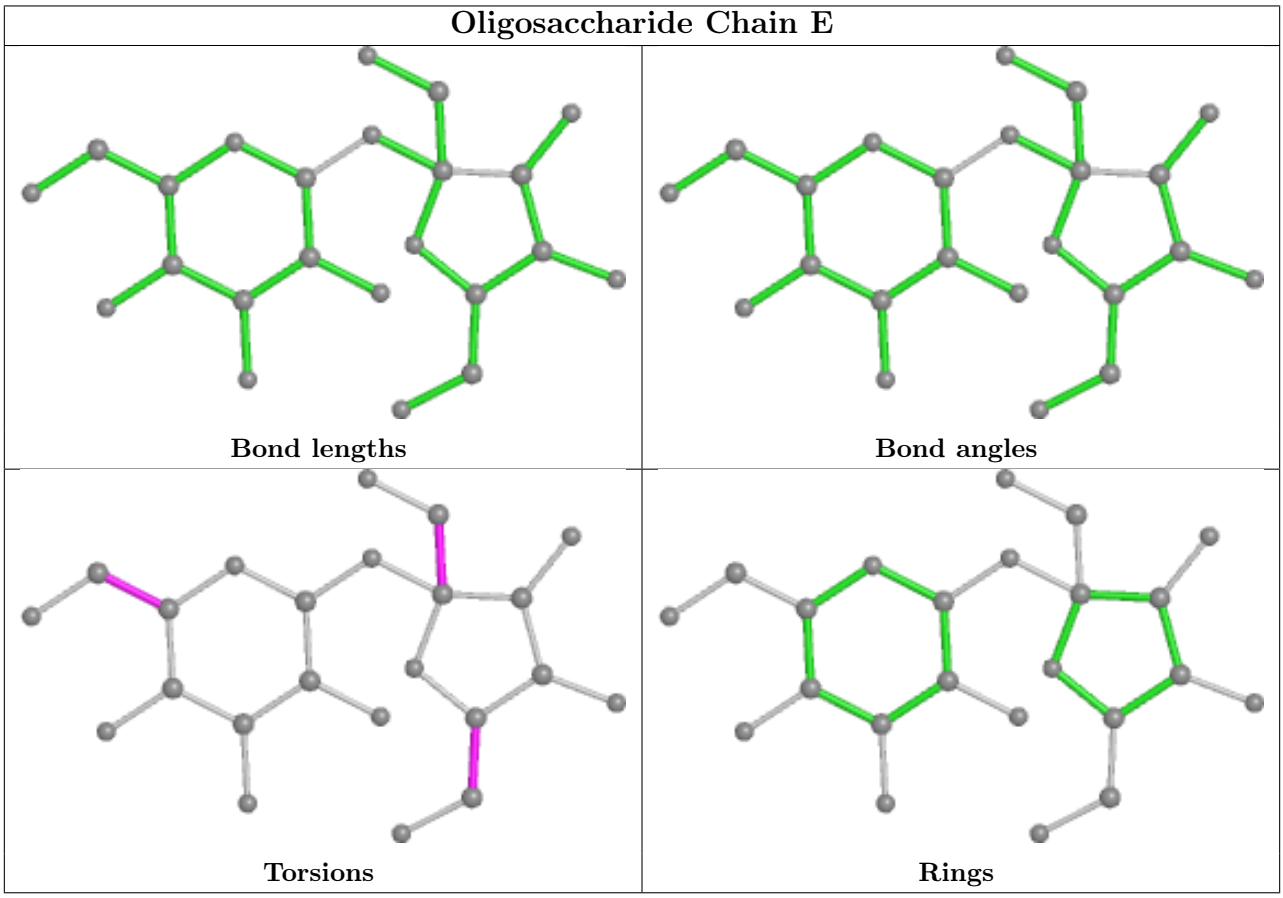
Mol	Chain	Res	Type	Atoms
5	E	2	FRU	O1-C1-C2-C3
5	E	2	FRU	O1-C1-C2-O2
5	E	2	FRU	O1-C1-C2-O5
5	E	2	FRU	C4-C5-C6-O6
5	E	2	FRU	O5-C5-C6-O6
5	E	1	GLC	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	2	FRU	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry (i)

14 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	NAG	A	886	1	14,14,15	0.55	0	17,19,21	0.72	0
6	NAG	A	795	1	14,14,15	0.50	0	17,19,21	1.14	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	NAG	A	762	1	14,14,15	0.57	0	17,19,21	0.87	1 (5%)
6	NAG	A	741	1	14,14,15	0.50	0	17,19,21	0.85	0
6	NAG	A	789	1	14,14,15	0.55	0	17,19,21	0.86	0
6	NAG	A	948	1	14,14,15	0.54	0	17,19,21	0.78	0
8	HEZ	A	4003	-	7,7,7	0.28	0	6,6,6	0.51	0
7	EDO	A	4001	-	3,3,3	0.42	0	2,2,2	0.37	0
7	EDO	D	4002	-	3,3,3	0.44	0	2,2,2	0.37	0
6	NAG	A	734	1	14,14,15	0.50	0	17,19,21	0.86	0
6	NAG	A	730	1	14,14,15	0.58	0	17,19,21	0.87	1 (5%)
6	NAG	A	776	1	14,14,15	0.54	0	17,19,21	0.80	0
6	NAG	A	892	1	14,14,15	0.52	0	17,19,21	0.72	0
6	NAG	A	839	1	14,14,15	0.62	0	17,19,21	0.88	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	A	886	1	-	2/6/23/26	0/1/1/1
6	NAG	A	795	1	-	2/6/23/26	0/1/1/1
6	NAG	A	762	1	-	2/6/23/26	0/1/1/1
6	NAG	A	741	1	-	2/6/23/26	0/1/1/1
6	NAG	A	789	1	-	0/6/23/26	0/1/1/1
6	NAG	A	948	1	-	0/6/23/26	0/1/1/1
8	HEZ	A	4003	-	-	2/5/5/5	-
7	EDO	A	4001	-	-	1/1/1/1	-
7	EDO	D	4002	-	-	0/1/1/1	-
6	NAG	A	734	1	-	0/6/23/26	0/1/1/1
6	NAG	A	730	1	-	0/6/23/26	0/1/1/1
6	NAG	A	776	1	-	0/6/23/26	0/1/1/1
6	NAG	A	892	1	-	2/6/23/26	0/1/1/1
6	NAG	A	839	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	795	NAG	O5-C5-C6	2.45	111.05	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	762	NAG	O5-C5-C6	2.39	110.95	107.20
6	A	795	NAG	C2-N2-C7	2.32	126.20	122.90
6	A	730	NAG	O5-C5-C6	2.04	110.40	107.20
6	A	839	NAG	O5-C1-C2	2.00	114.45	111.29

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	839	NAG	C1-C2-N2-C7
6	A	886	NAG	C8-C7-N2-C2
6	A	892	NAG	O5-C5-C6-O6
6	A	795	NAG	C8-C7-N2-C2
6	A	795	NAG	O7-C7-N2-C2
6	A	886	NAG	O7-C7-N2-C2
6	A	892	NAG	C4-C5-C6-O6
6	A	741	NAG	C4-C5-C6-O6
8	A	4003	HEZ	C3-C4-C5-C6
6	A	741	NAG	O5-C5-C6-O6
8	A	4003	HEZ	O1-C1-C2-C3
6	A	762	NAG	C4-C5-C6-O6
6	A	762	NAG	O5-C5-C6-O6
7	A	4001	EDO	O1-C1-C2-O2
6	A	839	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	795	NAG	1	0
6	A	839	NAG	4	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	304/317 (95%)	0.44	20 (6%)	18	17	11, 34, 72, 122	0
2	B	181/184 (98%)	0.43	13 (7%)	15	14	18, 46, 78, 90	0
3	C	214/214 (100%)	-0.05	2 (0%)	84	83	9, 30, 70, 83	0
4	D	221/229 (96%)	-0.33	1 (0%)	91	90	7, 20, 61, 84	0
All	All	920/944 (97%)	0.14	36 (3%)	39	38	7, 32, 73, 122	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	129	ALA	23.5
1	A	128	GLY	10.4
1	A	127	VAL	9.3
1	A	194	GLY	8.0
1	A	195	SER	7.5
1	A	126	CYS	6.7
1	A	125	LEU	5.1
1	A	196	CYS	5.0
1	A	462	ASN	5.0
2	B	1105	ASP	4.8
1	A	210	PHE	3.9
1	A	87	VAL	3.8
2	B	1001	LYS	3.8
1	A	356	ASN	3.7
2	B	1181	LYS	3.5
2	B	1123	GLY	3.1
2	B	1019	SER	3.0
1	A	463	ASN	2.9
1	A	490	LYS	2.8
1	A	88	ASN	2.7
2	B	1106	THR	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	1104	SER	2.6
4	D	3001	GLU	2.4
1	A	89	VAL	2.4
1	A	410	GLY	2.3
2	B	1162	LEU	2.2
3	C	2001	ASP	2.2
2	B	1088	ASP	2.1
3	C	2190	LYS	2.1
2	B	1125	SER	2.1
1	A	83	GLU	2.1
1	A	461	SER	2.1
1	A	240	THR	2.0
2	B	1096	LEU	2.0
2	B	1020	GLN	2.0
2	B	1089	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

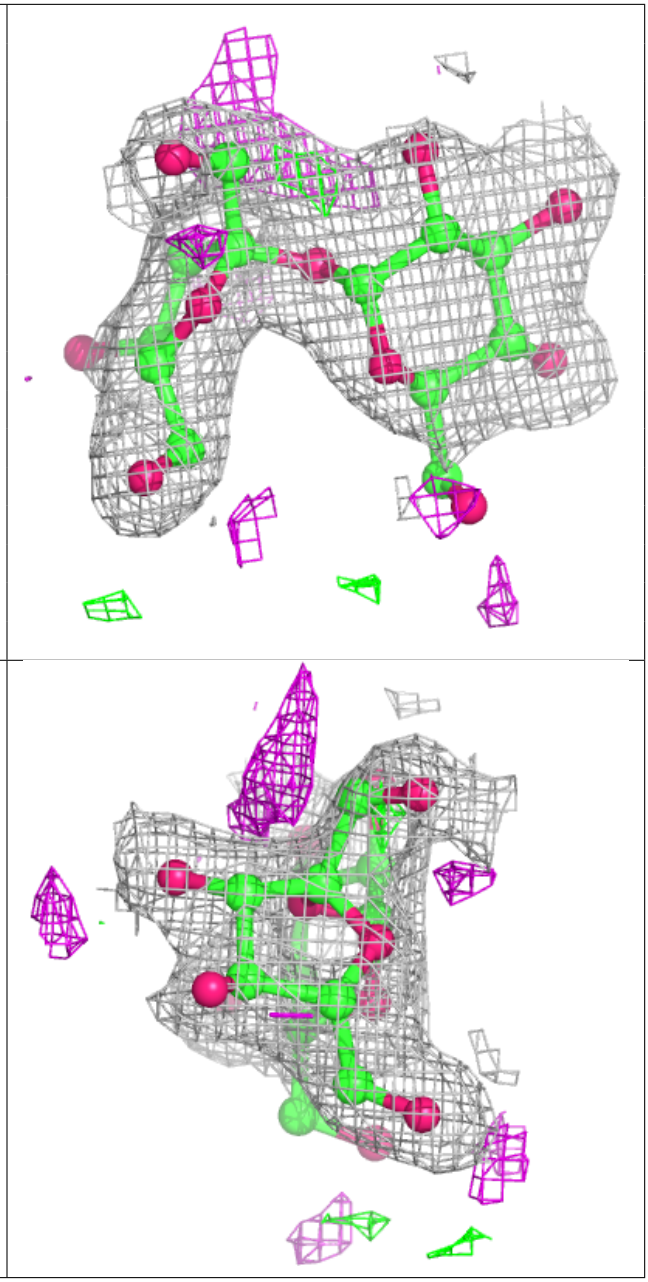
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	FRU	E	2	12/12	0.72	0.25	71,75,79,81	0
5	GLC	E	1	11/12	0.83	0.21	60,62,68,69	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	EDO	A	4001	4/4	0.15	1.37	323,324,330,332	0
6	NAG	A	839	14/15	0.20	0.40	503,529,544,546	0
8	HEZ	A	4003	8/8	0.23	2.50	371,376,382,385	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NAG	A	948	14/15	0.37	1.27	386,435,470,472	0
6	NAG	A	892	14/15	0.38	0.60	359,402,439,443	0
6	NAG	A	730	14/15	0.43	0.53	585,602,630,632	0
6	NAG	A	734	14/15	0.46	0.84	502,528,545,549	0
6	NAG	A	795	14/15	0.48	0.89	386,398,423,424	0
6	NAG	A	762	14/15	0.51	1.03	307,331,362,363	0
6	NAG	A	776	14/15	0.51	1.08	404,423,430,432	0
6	NAG	A	741	14/15	0.59	0.52	570,617,651,654	0
6	NAG	A	886	14/15	0.65	0.71	260,289,303,311	0
6	NAG	A	789	14/15	0.67	0.42	532,552,571,579	0
7	EDO	D	4002	4/4	0.89	0.20	53,54,55,55	0

6.5 Other polymers (i)

There are no such residues in this entry.